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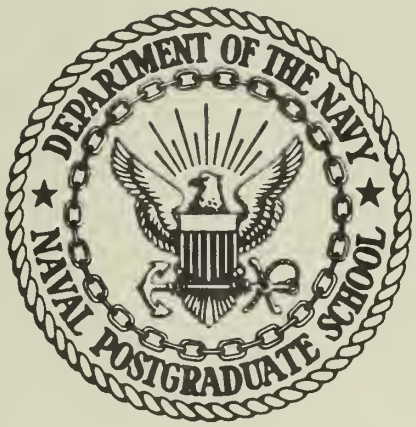

PREDICTED PARAMETER UNCERTAINTIES FOR

LEAST SQUARES ANALYSIS OF A SINGLE EXPONENTIAL DECAY WITH A CONSTANT BACKGROUND RATE

by

G. W. Rodeback

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ABSTRACT:

The decay constant and initial activity for a single exponential decay, together with a constant background activity, are assumed to be the three adjustable parameters for a least squares fit of experimental data. The expected variances of these three parameters are predicted mathematically for the general case where it is assumed that experimental decay counts with inherent statistical uncertainty are collected in successive equal time intervals of negligible uncertainty. Comparisons of a parameter uncertainty with respect to the time interval, number of intervals and background activity are based on a fixed "confidence interval" for the parameter. Assumed background rates are expressed as fractions of the initial decay activity. The results can be simply applied to arbitrarily assumed values of decay constant and initial activity.

This work was supported in part by the Office of Naval Research through the Naval Postgraduate School Research Foundation Program.

INTRODUCTION

The experimenter measuring a radioactive decay very often must decide both the sizes of the time intervals for each group of counts recorded and the total number of groups of counts to be recorded. Analysis of the data then permits determination of the decay activity, the decay constant, and the background activity with hopefully sufficient precision for one or more of these quantities. It is hoped that this paper may be useful in making the above decisions for the measurement of a single decay plus background, where the multi-scalar mode of a multi-channel analyser is often employed, and where the data are least-squares analysed. Only statistical counting errors are treated. It is assumed that decay counts are recorded successively in equal time intervals of negligible uncertainty. The least squares analysis of these data then yields the calculated values of the three parameters: decay constant, initial activity, and constant background activity. The unbiased estimates of the variances (standard deviations squared) of the above parameters are also given by least squares analysis.

Prediction analysis[1] applied to the type of experiment stated above, yields the predicted values of the three variances for assumed values of the three corresponding parameters for a given time interval and given number of data points. The values of these predicted variances are comparable to the average values which would be obtained if an actual experiment (with the above assumed values of parameters, time interval and number of points) were repeated a large number of times.

The numerical results obtained are used to make comparisons of the predicted uncertainties of any one of the parameters over large ranges of values of time interval and number of points. Assuming that approximate values of the parameters are known in advance, the results shown may then be used as a guide for the experimenter to make valid, practical decisions regarding time interval and number of points in order to achieve some particular desired accuracy in one or more of the parameters calculated by least squares analysis.

ANALYSIS

Some Pertinent Features of the Least Squares Analysis

The calculated total activity $\dot{n}$ in counts per unit time corresponding to what would be registered by a counting apparatus can be represented as,

$$\dot{n} = \dot{n}_o e^{-\lambda t} + \dot{n}_b$$

where t is the time, $\dot{n}_o$ and λ are the initial activity and decay constant of the exponential decay, and $\dot{n}_b$ is the constant background activity. Integration of the above, results in:

$$n_c = (\dot{n}_o/\lambda)(1 - e^{-\lambda t}) + \dot{n}_b t$$

where n_c represents the calculated number of counts corresponding to those registered during the time t.

Now if counts are registered during equal time intervals τ starting at $t = 0$, then $t_i = i\tau$, $(i = 0, 1, \ldots\ldots Q)$, represents the beginning time of the i'th counting interval, there are a total of $M = Q + 1$ counting intervals and thus M experimental points. Applying the above we have

$$n_i = (\dot{n}_o/\lambda)\left[e^{-i\lambda\tau}(1 - e^{-\lambda\tau}) + (\dot{n}_b/\dot{n}_o)\lambda\tau\right] \qquad (1)$$
$$i = 0, 1, \ldots\ldots Q$$

where n_i represents the calculated value of the number of counts in the i'th counting interval. In later portions of the paper the ratio of $\dot{n}_b$ to $\dot{n}_o$ is expressed by the symbol ϵ , ie. $\epsilon = \dot{n}_b/\dot{n}_o$. It will be assumed that λ , $\dot{n}_o$ and $\dot{n}_b$ represent the calculated values of the three parameters based on a least squares analysis of M experimental points. Thus, n_i in Eq. (1) is the least-squares-calculated value of counts for the i'th time interval.

An actual measurement over the M time intervals of width τ , records N_i counts in the i'th interval, subject to statistical fluctuations. Thus the estimate of the standard deviation of N_i is given by $\sqrt{N_i}$. A least squares analysis[2,3,4] of the M points determines those

values of the parameters λ , $\dot{n}_o$, $\dot{n}_b$ which minimize the sum of the weighted squares of the residuals given by $S = \sum_{i=o}^{Q} (1/N_i)(N_i - n_i)^2$. The term $(N_i - n_i)$ is the i'th residual and $1/N_i$ is the "weight" of the i'th point. If a particular experiment with M points were repeated many times, the mean value of S would be (M - 3). (M - 3) is the number of "degrees of freedom" - in general the number of degrees of freedom (denoted symbolically by n - p) equals the number of points minus the number of parameters.

It is assumed that an iterative least squares analysis has been made (usually by computer), whereby the function in Eq. (1) is linearized with respect to the parameters λ , $\dot{n}_o$ and $\dot{n}_b$ for each i'th point. The linearization involves the following quantities for each point:

$$a_i = \frac{1}{\sqrt{N_i}} \frac{\partial n_i}{\partial \lambda} \quad , \qquad b_i = \frac{1}{\sqrt{N_i}} \frac{\partial n_i}{\partial \dot{n}_o} \quad , \qquad c_i = \frac{1}{\sqrt{N_i}} \frac{\partial n_i}{\partial \dot{n}_b} \tag{2}$$

where each of the above partial derivatives is evaluated with the final (i.e., the last step in the iterative calculation) calculated values for λ , $\dot{n}_o$ and $\dot{n}_b$.

The symmetric three by three "coefficient matrix" C is constructed using the terms in Eqs. (2). The six different elements of C are given by:

$$C_{11} = \Sigma a_i^2 \qquad C_{22} = \Sigma b_i^2 \qquad C_{33} = \Sigma c_i^2$$

$$C_{12} = \Sigma a_i b_i \qquad C_{23} = \Sigma b_i c_i \qquad C_{31} = \Sigma c_i a_i \tag{3}$$

(The above summations are from i = 0 to i = Q.)

The elements of this matrix, together with the numerical values of the observed counts, are used to determine the calculated values of the three parameters.

Let $s(\lambda)$, $s(\dot{n}_o)$, $s(\dot{n}_b)$ represent the unbiased estimates of the standard deviations of λ , $\dot{n}_o$ and $\dot{n}_b$ respectively. The corresponding variances from the theory of least squares analysis are:

$$s^2(\lambda) = \left(\frac{S}{M - 3}\right) C_{11}^{-1} \quad , \quad s^2(\dot{n}_o) = \left(\frac{S}{M - 3}\right) C_{22}^{-1} \quad , \quad s^2(\dot{n}_b) = \left(\frac{S}{M - 3}\right) C_{33}^{-1} \tag{4}$$

The three matrix elements are the diagonal elements of the inverse coefficient matrix, i.e., C^{-1}. The term $S/(M - 3)$ which appears in each of the above expressions is called by some authors the "weighted variance of fit".[5]

Prediction of the Variances

The above discussion has briefly mentioned those features of the least squares analysis of actual data (as applied to the particular problem of single exponential decay plus constant background) which are pertinent to the main topic of this article, ie. the prediction of the parameter uncertainties. Prediction of the variances of the parameters comes under the general subject of Prediction Analysis which is a general method for predicting the uncertainties of results that should be obtained from a proposed experiment[6].

Referring to Eqs. (4) we note that each of the variances has the $S/(M - 3)$ factor. As mentioned above, the mean value of S is $M - 3$. Thus, the mean value of the entire factor (ie. the weighted variance of fit) is unity. This is the average value of the factor which should be obtained if the experiment were to be repeated many times. Accordingly, the predicted variances are defined to be:

$$\hat{s}^2(\lambda) = \hat{C}^{-1}_{11} \quad , \qquad \hat{s}^2(\dot{n}_o) = \hat{C}^{-1}_{22} \quad , \qquad \hat{s}^2(\dot{n}_b) = \hat{C}^{-1}_{33} \tag{5}$$

Some of the notation of the preceding reference[6] is used here, where the caret ($\wedge$) denotes the predicted value of a quantity. Thus the diagonal elements of the predicted inverse coefficient matrix appear in the above expressions. The elements of the predicted coefficient matrix and those of the predicted inverse coefficient matrix are formed as follows:

1. Arbitrary values of λ , $\dot{n}_o$ and $\dot{n}_b$ are assumed. They will still be denoted by the above symbols in this discussion.
2. Eq. (1) is used to evaluate the expressions in Eq (2) together with the substitution of n_i for N_i in Eq. (2).
3. The elements in Eq. (3) are now formed using the predicted versions of Eq. (2). Thus the predicted coefficient matrix can be formulated.
4. Desired elements of the predicted inverse coefficient matrix are now evaluated from the predicted coefficient matrix.

The results of carrying out the above steps to determine the predicted variances of Eq. (5) are expressed most simply by the following summarization where first we have for the squares of the predicted fractional standard deviations:

$$\frac{\hat{s}^2(\lambda)}{\lambda^2} = \left(\frac{\lambda}{\dot{n}_o}\right) G \ , \qquad \frac{\hat{s}^2(\dot{n}_o)}{\dot{n}_o^2} = \left(\frac{\lambda}{\dot{n}_o}\right) A \ , \qquad \frac{\hat{s}^2(\dot{n}_b)}{\dot{n}_b^2} = \left(\frac{\lambda}{\dot{n}_o}\right) B \qquad \text{(6a, b, c)}$$

(6a) (6b) (6c)

With P defined by the equation $P = \lambda\tau$; also $\epsilon = \dot{n}_b/\dot{n}_o$ and $Q = M - 1$, we have:

$$G = 1\Big/\left\{ [aa] + \frac{2[ab][bc][ca] - [bb][ac]^2 - [cc][ab]^2}{[bb][cc] - [bc]^2} \right\} \qquad (7a)$$

$$A = 1\Big/\left\{ (1 - e^{-P})^2 \left[[bb] + \frac{2[ab][bc][ca] - [cc][ab]^2 - [aa][bc]^2}{[cc][aa] - [ca]^2} \right] \right\} \qquad (7b)$$

$$B = 1\Big/\left\{ (\epsilon^2 P^2) \left[[cc] + \frac{2[ab][bc][ca] - [aa][bc]^2 - [bb][ca]^2}{[aa][bb] - [ab]^2} \right] \right\} \qquad (7c)$$

and with the use of the two defining equations,

$$N(i) = Pe^{-P} - (1 + iP)(1 - e^{-P}) \ , \quad D(i) = \epsilon P + (1 - e^{-P})e^{-iP}$$

Eqs. (7) are evaluated with:

$$[aa] = \Sigma e^{-2iP} N^2(i)/D(i) \ , \ [bb] = \Sigma e^{-2iP}/D(i) \ , \ [cc] = \Sigma 1/D(i)$$

$$[ab] = \Sigma e^{-2iP} N(i)/D(i) \ , \ [bc] = \Sigma e^{-iP}/D(i) \ , \ [ca] = \Sigma e^{-iP} N(i)/D(i)$$

(The above summations are from $i = 0$ to $i = Q$)

RESULTS

A specific value of $P = \lambda\tau = \tau/(1/\lambda)$ denotes the magnitude of the time interval measured in units of mean-lives. $(1/\lambda$ is the mean-life in units of time corresponding to λ ; the corresponding half-life is $\ln 2/\lambda)$. From Eqs. (6) and (7) we note that G, A and B are functions only of ϵ , P and M; thus when ϵ , P and M are specified the quantities G, A and B can be completely determined. Exact numerical values for these quantities have

been calculated for representative values of ϵ, P and M using the IBM 360 computer. The above expressions for G, A and B are particularly suited for computer calculation since for given values of ϵ and P, each additional term in the summations (such as [aa], [ab], etc.) corresponds effectively to a new value of M. Accordingly the computer output is programmed to render values of G, A and B for all possible values of M up to the maximum value specified in the input.

Assuming that the predicted variances are a valid measure of the uncertainties to be expected in the parameters, a study of G, A and B with respect to ϵ, P and M can be used to draw some useful qualitative conclusions regarding predicted accuracy. And when numerical values are chosen for λ and $\dot{n}_o$, the predicted fractional standard deviations (and hence the predicted variances and standard deviations) may be determined quantitatively.

For example, with assumed values of $\epsilon = 0.1$, $P = 1/200$, calculated values of G, A and B are plotted versus MP on Fig. 1. The numerical value of MP denotes the overall measurement time in mean-lives corresponding to M points. The abcissa on all subsequent Figures except Fig. 3 will be MP. Although the values of MP are discrete, the results are plotted as continuous curves. Note that for given values of λ and $\dot{n}_o$, every different combination of values of ϵ, P, M constitutes a unique experiment. In Fig. 2, G is shown versus MP for $\epsilon = 0.1$, 0.5 and 1.0 where $P = 1/200$. On the basis of these results we may say as expected, that for any given λ and $\dot{n}_o$ the predicted fractional standard deviations of all the parameters decrease as M increases (ie. as total counting time increases) and that the greater the amount of background compared to the initial activity, the larger the fractional standard deviation for λ. Exact comparisons of fractional standard deviations for different cases may be made with the above results if desired.

For a numerical illustration we choose a decay whose mean-life is 1032 hours (43 days) and whose initial activity is 72,000 counts/hour with one tenth of that as the background activity, ie. 7,200 counts/hour. For a counting interval of 1/200'th of a mean-life (5.16 hours) and a total counting time of 0.3 mean-lives (12.9 days), $G = 3.85 \times 10^5$ from Fig. 1 or Fig. 2. Applying Eq. (6a) we find that $\hat{s}^2(\lambda)/\lambda^2 = 5.2 \times 10^{-3}$; so $\hat{s}(\lambda)/\lambda = 7.2 \times 10^{-2}$ and $\hat{s}(\lambda) = 7.2\ 10^{-2}/1032 = 6.8 \times 10^{-5}$ hr.$^{-1}$. Thus, 7.2% fractional standard deviation is predicted for the determination of λ in the above experiment.

Let us again consider the least squares analysis of data for a given experiment. Repetition of this experiment would yield a distribution in the values of each of the calculated parameters. If these were normal distributions then one could say for one of the parameters (we shall use λ as an example) that 68.3% of the calculated values of λ would fall within $\pm s(\lambda)$ of the true value of λ, where $s(\lambda)$ is the unbiased estimate of the standard deviation of λ obtained from one of the sets of data. In general for n - p degrees of freedom, the parameters have a "t-distribution" rather than a normal distribution. For n - p degrees of freedom, values of $t_{.159,n-p}$ are those values of t for which there is a 68.3% probability that calculated values of λ will fall within $\pm s(\lambda)t_{.159,n-p}$ of the true value of λ. The total interval mentioned above is referred to as the 68.3% confidence interval. (Note that .159 = (1 - .683)/2 .) The larger n - p becomes the more closely the t-distribution approaches the normal distribution. For example $t_{.159,20} = 1.03$ and $t_{.159,\infty} = 1$. It will be assumed then that a comparison of $\hat{s}(\lambda)t_{.159,n-p}$ (and similarly for the other parameters) will give a valid comparison of the predicted uncertainties of the parameters for the assumed values of ϵ, M, and P. For the results shown in Figs. 1 and 2, comparisons without the t values are valid since all the corresponding values of n - p are 20 or greater. For the purpose of valid comparison we now replace the predicted standard deviations in Eqs. (6) with the product of $t_{.159}$ and the standard deviations (the product is half the 68.3% confidence interval) resulting in:

$$\left[\frac{\hat{s}(\lambda)}{\lambda}\right]^2 = \left(\frac{\lambda}{\dot{n}_o}\right) Gt^2_{.159}, \quad \left[\frac{\hat{s}(\dot{n}_o)}{\dot{n}_o}\right]^2 = \left(\frac{\lambda}{\dot{n}_o}\right) At^2_{.159}, \quad \left[\frac{\hat{s}(\dot{n}_b)}{\dot{n}_b}\right]^2 = \left(\frac{\lambda}{\dot{n}_o}\right) Bt^2_{.159} \qquad (8a, b, c)$$

(8a) (8b) (8c)

The $t^2_{.159}$ values of Fig. 3 are based on a linear interpolation from tables[7,8]. Only uncertainties in λ are considered in the results that follow. Figs. 4 and 5 are plots of $Gt^2_{.159}$ versus MP for representative values of ϵ, P and M.

$Gt^2_{.159}$ versus MP is plotted on Fig. 4 for different values of P when $\epsilon = 0.01$. From inspection of these curves it becomes apparent that the experimenter may achieve good precision for λ by choosing the counting interval to be about ½ of a mean-life and by collecting data for a total of about 10 mean-lives. The cost in additional effort of using a counting interval as small as 1/10 of a mean-life would not produce a worthwhile

improvement in precision, nor would counting for any longer total time appreciably improve the precision.

$Gt^2_{.159}$ versus MP is plotted on Fig. 5 where $P = \frac{1}{2}$, over a range of values of assumed background relative to $\dot{n}_o$. The conclusion reached in the above paragraph regarding total time of counting still appears to be valid provided the background is not too high. Even for $\epsilon = 0.2$, the fractional standard deviation in λ for 10 mean-lives total counting time is only 10% higher than for counting a total of 20 mean-lives. The dotted curve included in Fig. 5 is of interest. This was obtained from an analysis of a different case where no background activity is assumed. For this case Eq. (1) would not have the $\dot{n}_b$ term at all and only the parameters λ and $\dot{n}_o$ would be calculated. The condition $\epsilon = 0$ defines a particular value of $\dot{n}_b$ for the three-parameter case; this results in larger uncertainties for λ compared to the two-parameter case, when the total measuring time is less than 12 mean-lives.

The computer program devised for the case treated in this paper has been applied to a large range of values of ϵ, P and M of practical interest. Representative values of ϵ, P and M were chosen for the results shown in Figs. 1, 2, 4, and 5. It is seen from Figs. 4 and 5 that if desired, the limiting values of the standard deviations (or half-confidence intervals) can be approached by choosing M sufficiently large.

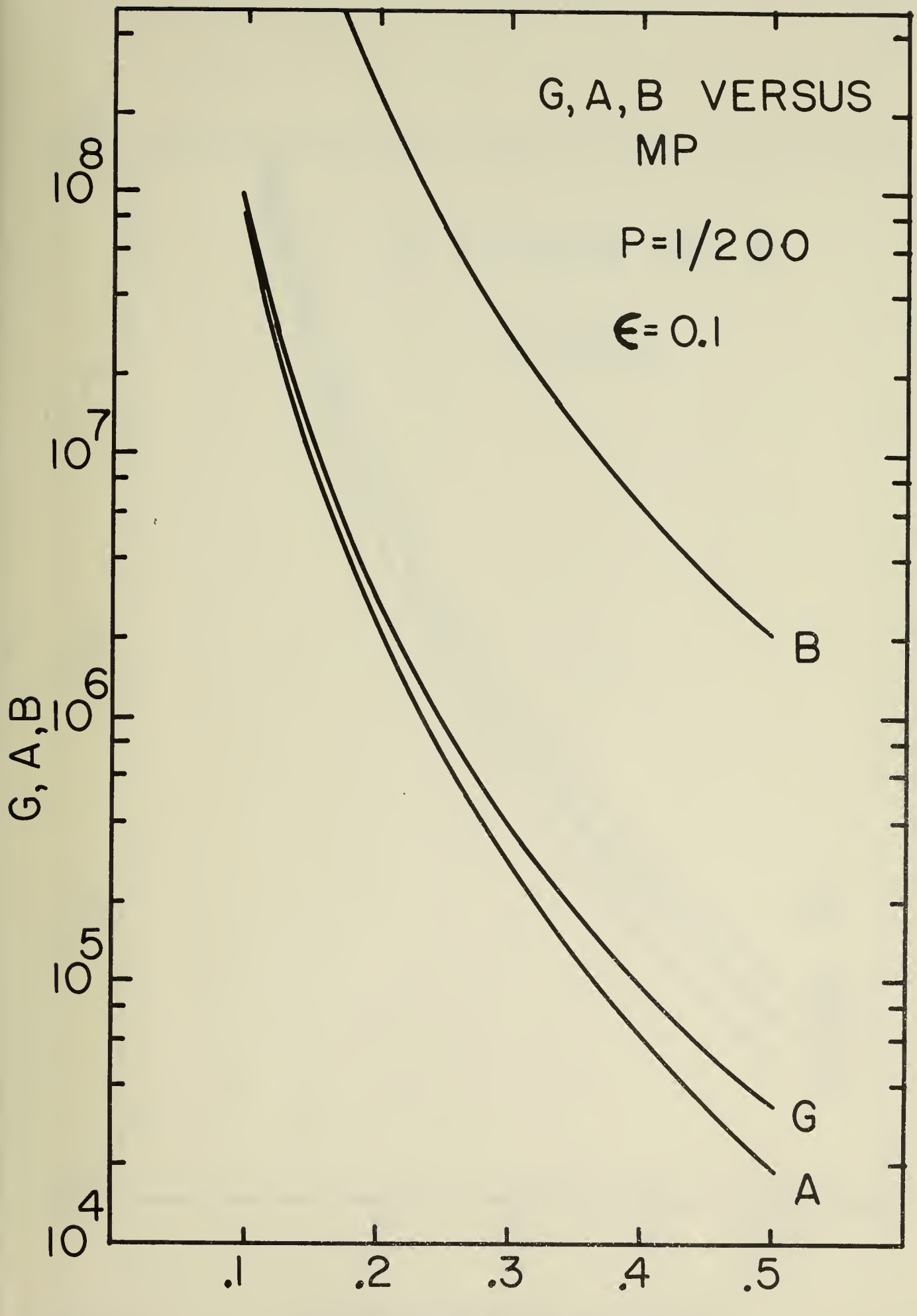

G, A, B VERSUS
MP
P=1/200
ϵ=0.1
B
G
A
G, A, B
10^8
10^7
10^6
10^5
10^4
.1
.2
.3
.4
.5
MP (MEAN-LIVES)

FIG. 1

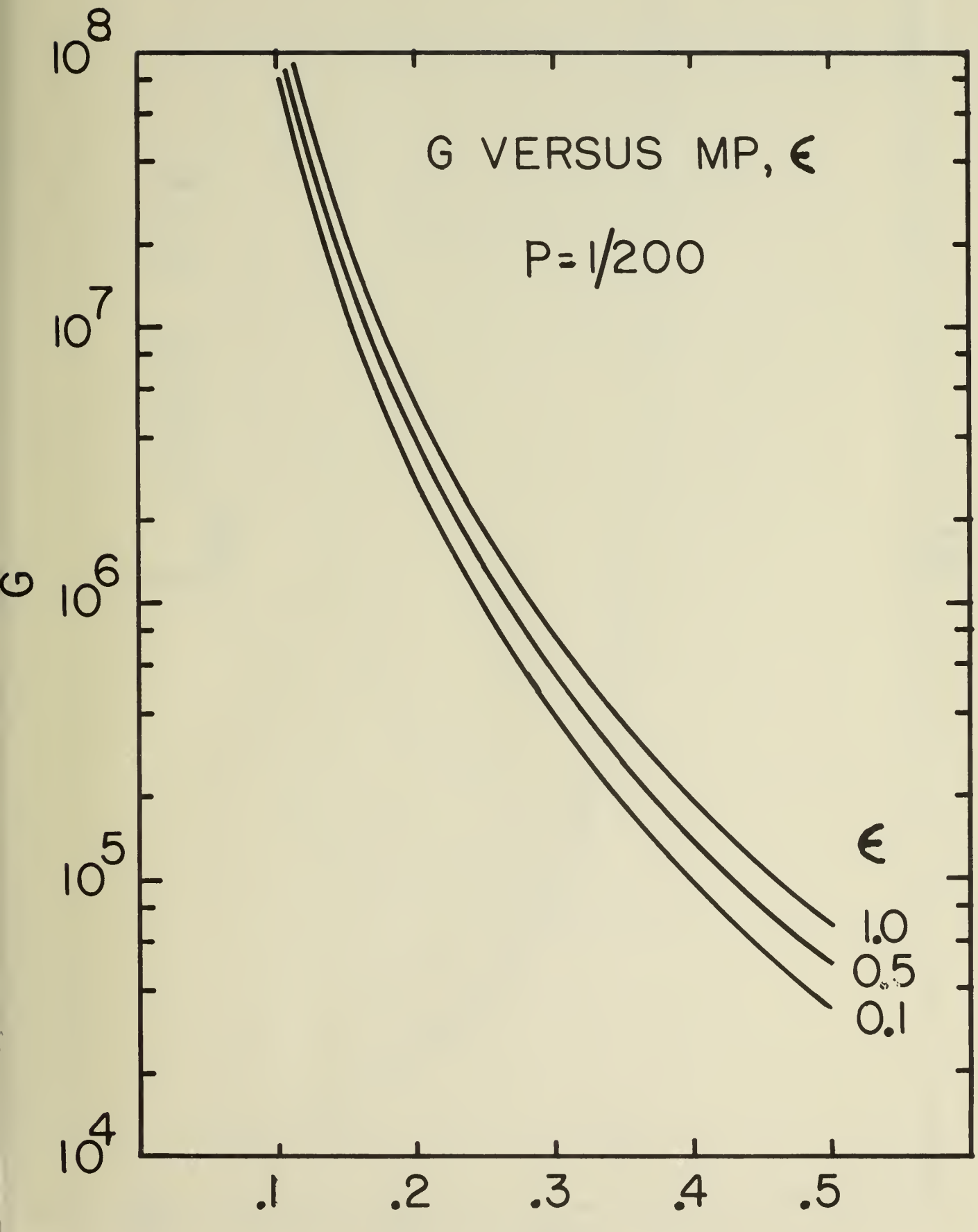

G VERSUS MP, ϵ
P = 1/200
G
10^8
10^7
10^6
10^5
10^4
.1
.2
.3
.4
.5
MP (MEAN-LIVES)
ϵ
1.0
0.5
0.1

FIG. 2

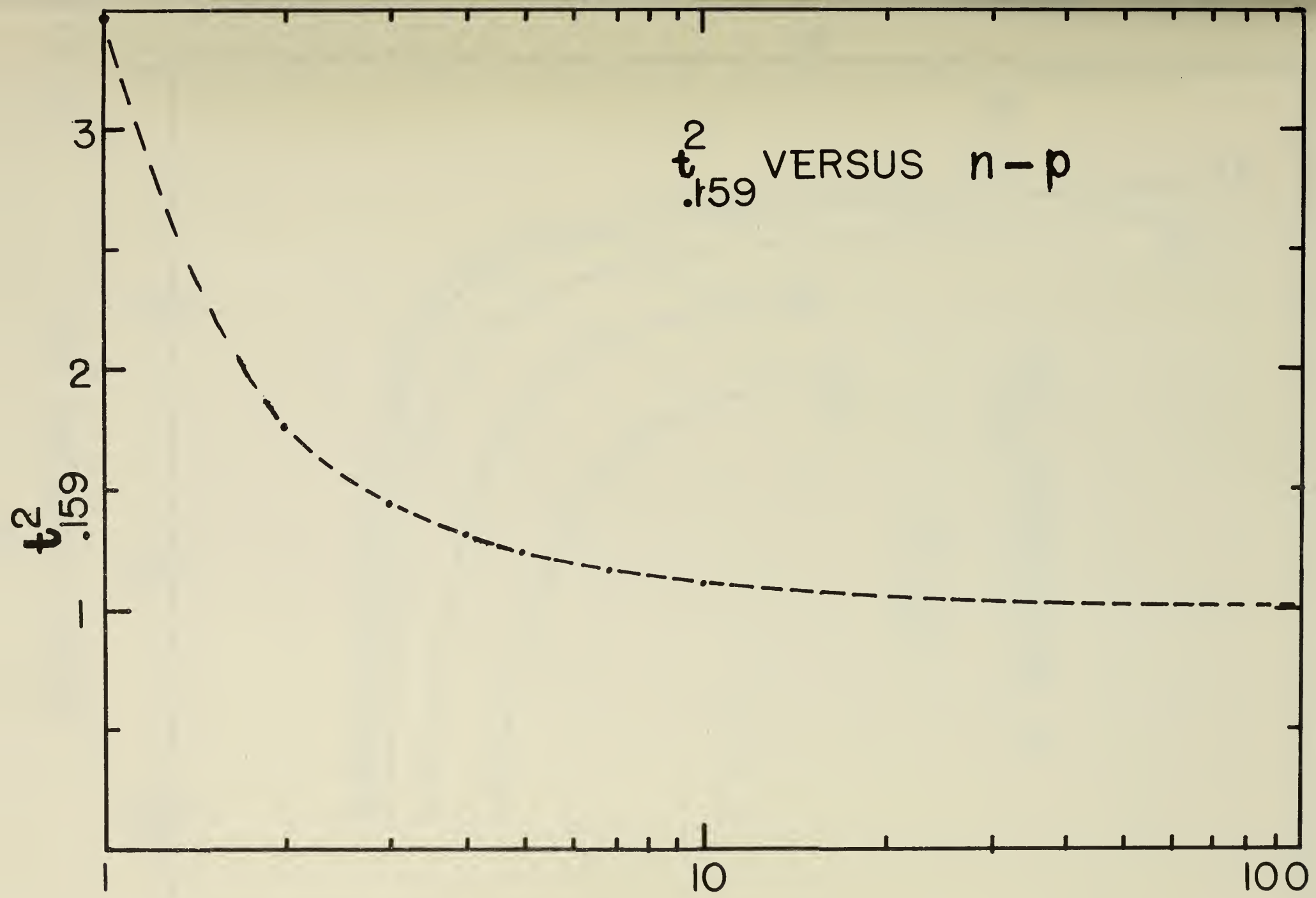


FIG. 3

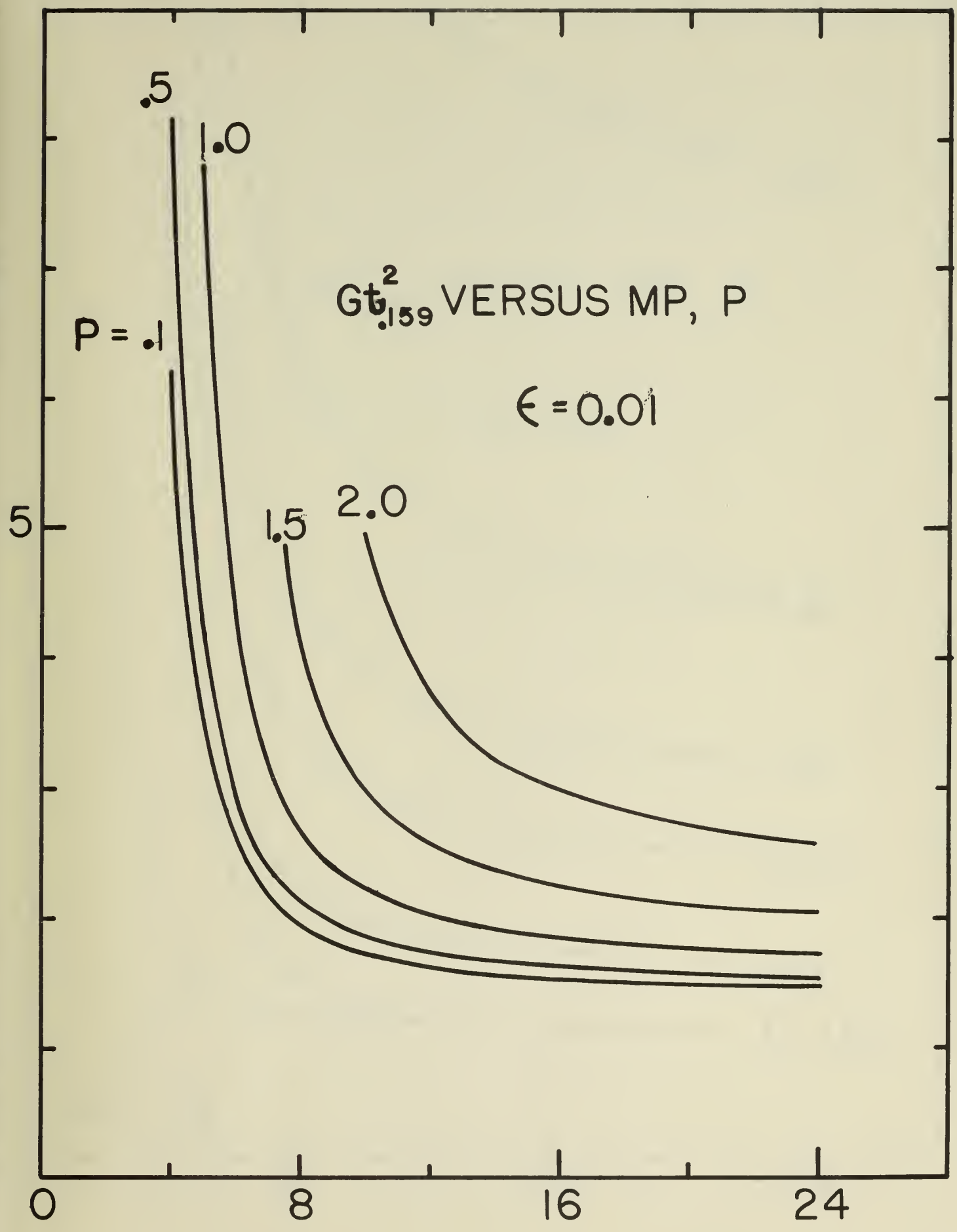

.5
1.0
P = .1
$Gt^2_{.159}$ VERSUS MP, P
$\epsilon = 0.01$
1.5
2.0
5
0
8
16
24
MP (MEAN-LIVES)

FIG. 4

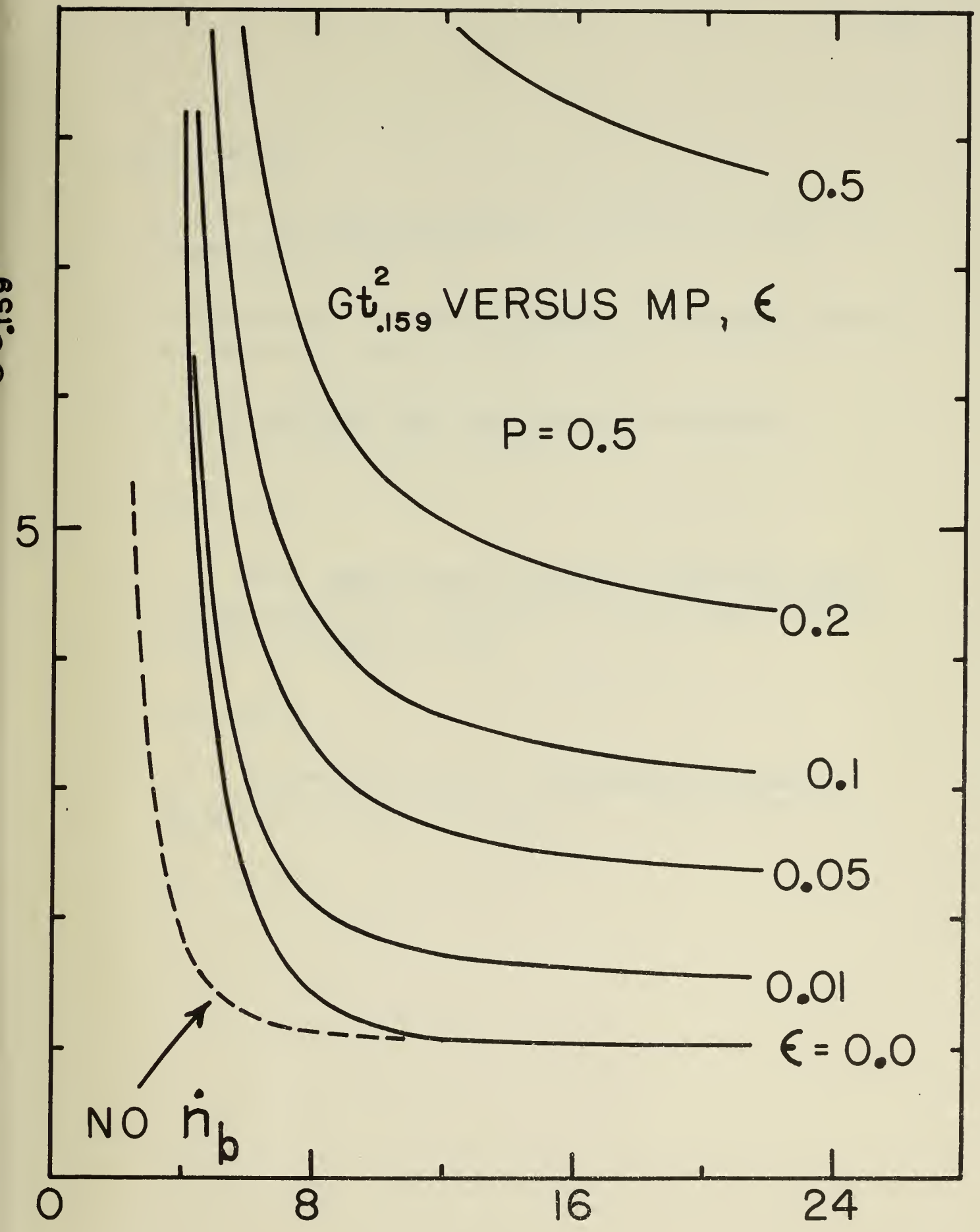
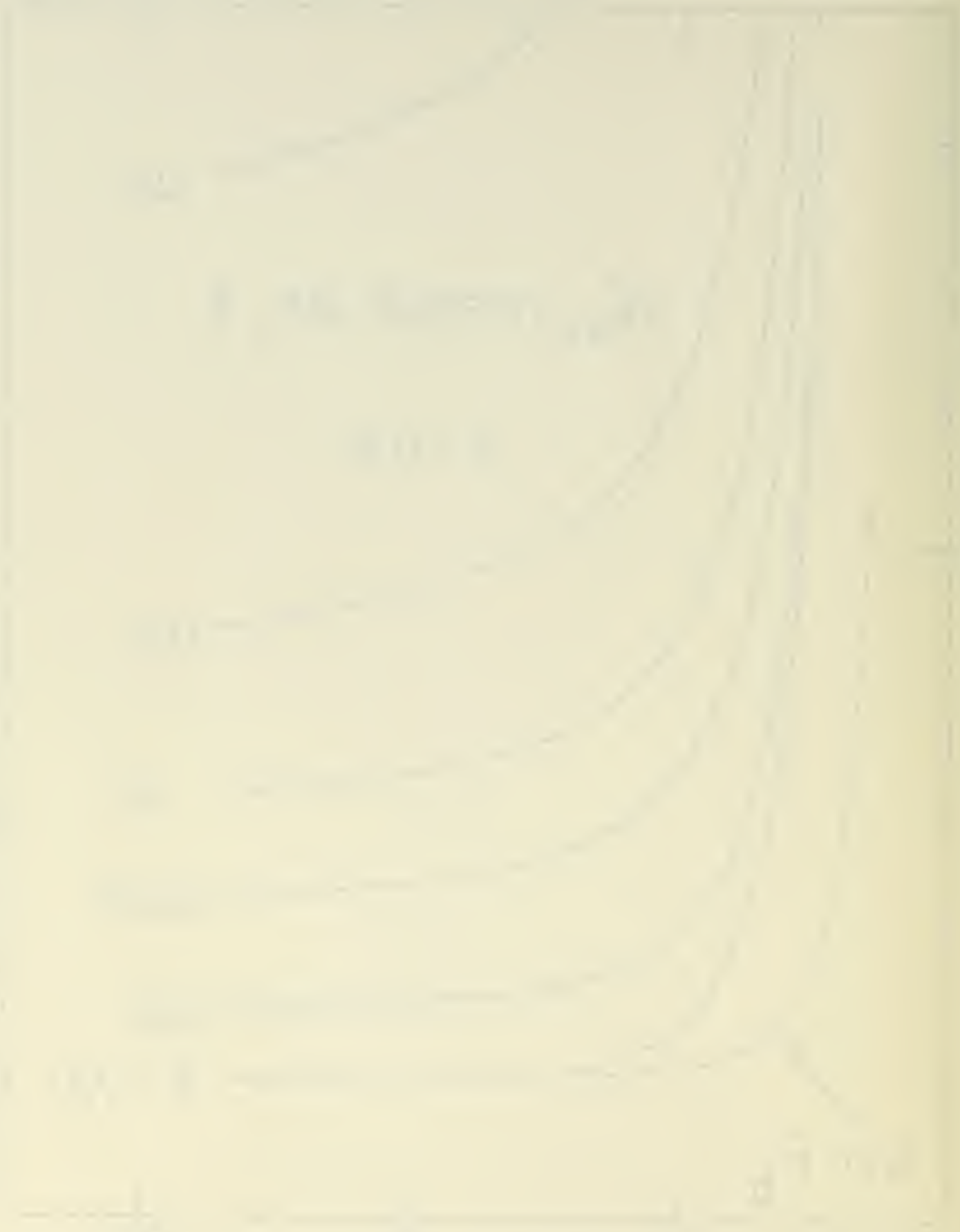


FIG. 5 MP (MEAN-LIVES)



LIST OF FOOTNOTES

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8 Ref. 1, p. 61

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13. ABSTRACT

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Variance						
Standard Deviation						